

1-Octadecanol
112-92-5 | DTXSID8026935

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 2950 L/kg

Global applicability domain: Outside

Local applicability domain index: 2.82e-01

Confidence level: 5.54e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2,4-DB 2-butoxyethyl ester</div> <div>Measured: 501</div> <div>Predicted: 1980</div>	<div>Image not found</div> <div>Dihexyl phthalate</div> <div>Measured: 52500</div> <div>Predicted: 23600</div>	<div>Image not found</div> <div>Fenoxycarb</div> <div>Measured: 1000</div> <div>Predicted: 1780</div>
<div>Image not found</div> <div>Fenoxycarb</div> <div>Measured: 1000</div> <div>Predicted: 1780</div>	<div>Image not found</div> <div>Bromoxynil octanoate</div> <div>Measured: 10000</div> <div>Predicted: 4120</div>	<div>Image not found</div> <div>Dichlorprop butoxyethyl ester</div> <div>Measured: 1000</div> <div>Predicted: 1310</div>